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# FINAL PROGRESS REPORT

Stephanos Venakides, Duke University

Grant DAAD19-99-1-0132

## WAVE PROPAGATION IN LINEAR AND NONLINEAR PHOTONIC BAND-GAP MATERIALS

### Abstract

1. Numerical Codes and Analysis: Simulation and analysis of 2D resonant phenomena in photonic crystal slabs through the study of dispersion relations of bulk medium and surface waves along the crystal using the boundary integral method. Development of 3D boundary element code for EM scattering off photonic crystal slabs. Development of 2D FDTD code that includes nonlinearities and use in studying resonant phenomena.
2. Nonlinear Effects: Derivation of the solution of the initial value problem of the small dispersion Nonlinear Schrödinger equation in the semi-classical limit. Study of 1:3 resonance in PBG circuit analogue.
3. Constrained optimization of photonic crystal structures. Determination of the geometry that optimizes a certain resonance under given geometric constraints.

## Background Information on Photonic Crystals and Statement of the Problem Studied

The goal of manipulating the optical properties of materials has arisen in the last decade. It is widely expected that progress in this area will produce great advancement in fields including lasers, high speed computers and spectroscopy. *Photonic Crystals* are combinations of two different dielectric materials arranged periodically in space, such as a spatially periodic array of rods or spheres of one type of dielectric material embedded in a different host material. As a result of the difference in the dielectric properties of the two materials, it has been found that photonic crystals may display *Photonic Bandgaps* (PBG's), i.e. frequency intervals for which the propagation of electromagnetic waves is forbidden in all directions within the spatially periodic dielectric structure. The existence of band-gaps is basically due to the coherent multiple scattering and interference of waves in the periodic structure. Thus, in bandgap frequencies, the photonic crystal is a practically lossless, perfect reflector that can be used to affect the radiative dynamics within an optical structure and have a dramatic technological impact. For example, it is well known that antenna efficiency decreases due to losses from surface waves on the antenna substrate. Such losses are avoided when the

substrate is a PBG material that the surface wave cannot penetrate. The increase of the antenna efficiency is very significant. A most important application is the reduction of spontaneous emission that could greatly enhance laser efficiency. Photonic crystals may play a significant role in the development of optical switches that will provide all optical communications. PBG reflectors could also be used in a direct defense application to deflect laser beams coming from any direction. The use of PBG materials with induced defects is very promising. Point defects in the PBG structure generate robust localized states, while defects along a line serve as optical waveguides that transmit an optical signal without the restriction on the bending angle that traditional optical fibers display. Random defects are expected to play the same role that impurities play in semiconductors. Last but not least, resonant behavior of the photonic crystal may be utilized for constructing photonid resonators at the nano/micro scale.

The broad goals of the present project have been:

1. Development of 2D and 3D numerical codes for the study of EM scattering by photonic crystal slabs as well as for identifying bound states and resonances.
2. Study of the effect of nonlinearity in periodic and optical media.
3. Inverse and optimization problems in photonic crystal structures.

## **Summary of most important results**

### **Numerical Codes and Analysis**

#### **2D EM transmission and resonance problems**

In collaboration with M. Haider and S. Shipman, we have completed a new fast 2D BEM code for simulating scattering by photonic crystal slabs. The code is significantly faster than the previous one developed in collaboration with M. Haider and V. Papanicolaou. The computational speed is achieved by using the separability of the terms in the expression for the periodic Green's function to define a set of new variables that lump influences from large sets of source points and are independent of the observation points. The new variables eliminate any duplication in the calculations making the assembling of the matrix more efficient and lead to a system of linear equations that has a banded coefficient matrix, as opposed to the dense matrix of our previous approach. The separability is in the propagation direction, thus the method favors period cells that are short in the transverse direction. Applying the code in photonic crystal slabs with a certain type of periodic defect in the structure that we called a channel defect, we observed resonance phenomena not only in the bandgaps but also in the bands. We originally detected these phenomena by observing accompanying transmission anomalies, and then verified that they occurred when our integral equations were near singular.

In collaboration with Shipman, we developed a mathematical theory of photonic crystal slab resonant behavior by examining the dispersion relation with real wavelength and

complex frequency (we are currently also complexifying the wavelength). The wavenumber appears in our formulation as the single period Bloch phase shift, that is the phase shift produced by the pseudoperiodic boundary condition. The fact that the domain of our integral equations is a compact subset of the strip that forms our periodic cell, forces the dispersion relation to be analytic, and allows us the analytic extension of "eigenmodes" into the complex frequency plane. We verify numerically the existence of complex resonant frequencies (given by zeroes of the determinant of our equations) using the argument principle.

We link transmission anomalies at real frequencies to the existence of nearby complex resonances. In fact, these resonances are on branches of the dispersion relation (curves on the complex plane parametrized by the real wavenumber) that emanate from the real axis into the complex frequency plane often staying close to the real axis. The smaller the imaginary part of the complex resonant frequency, the sharper the transmission anomaly in a scattering experiment with an incident wave of frequency equal to the real part of the resonant frequency.

In current work, we believe that we have identified the analytic source of the transmission anomaly and we will be able to reproduce its shape analytically.

### **Transmission through a 3D photonic crystal slab**

In collaboration with Andrew Barnes (PhD Dissertation, in progress), we have developed a 3D BEM code to simulate EM transmission through a 3D photonic crystal slab. Our code utilizes the periodicity of the structure by using the periodic Green's function (Ewald representation) and uses a well posed (Fredholm second kind) system leading to a stable solve. A lot of the work has gone into making the Green's function calculations efficient.

The code has been validated in two ways, firstly in the case of a flat slab, where the scattering problem is effectively 1D and can be solved by hand, and secondly in the case of the slab consisting of parallel cylinders, where results were verified by our 2D code.

### **FDTD code**

We have studied surface and bulk waves in a photonic crystal slab of the first project using both FDTD (finite difference time domain code) and BEM (see above). The disadvantage of FDTD is that it is slow to capture resonances accurately. It takes a lot of time for the resonant field to build up. Its great merits are that it is very efficient away from resonance, being able to cover a band of frequencies in the same time-based calculation, and that it can include nonlinearities.

In collaboration with C. Hale (PhD dissertation, in progress), we have developed a nonlinear 2D FDTD code, with which (1) we have verified results obtained earlier with our BEM code and (2) have carried out dynamic scattering numerical experiments linking observed field decay to the imaginary component of the dispersion relation obtained earlier through our frequency based BEM code. Work is in progress.

## Nonlinear Effects

### Study of nonlinear circuit analogues to transmission through nonlinear periodic media

In collaboration with A. Georgieva and T. Kriecherbauer, we have previously investigated traveling waves through a nonlinear inductor/capacitor circuit that is an analogue of a 1D periodic medium. We constructed traveling wave solutions through this nonlinear medium, at all nonresonant frequencies in the corresponding linear frequency bands. We found second harmonic generation near the resonance 1:2 at which an acoustic mode resonates with an optical mode. As the frequency is increased in solution space, from slightly below resonance to slightly above resonance, while a wave energy parameter is kept constant, the energy, almost entirely in the first harmonic at the outset, is necessarily transferred completely to the second harmonic. At the point at which the first harmonic vanishes, the second harmonic becomes identical with the optical mode.

We have investigated third harmonic generation at the resonance 1:3 under the present grant. We have derived the bifurcation equations that govern the phenomenon. We find that the topology in solution space differs between the 1:2 and 1:3 resonance. Indeed, third harmonic generation does not occur necessarily in solution space as one varies the frequency of a constant energy wave through its resonant value. We are in the process of studying the phenomenon further.

### The NLS equation

The NLS equation describes solitonic transmission in fiber optic communication and is generically encountered in propagation through nonlinear media. It will play a serious role in wave propagation through a photonic crystal. One of its most important aspects is the modulational instability that it displays. Regular wavetrains are unstable to modulation and break up to more complicated structures.

The NLS equation is solvable in theory by the method of inverse scattering, which utilizes spectral information of a linear operator, the Zakharov Shabhat (ZS) operator, associated with the unknown solution. In the first step of the method, the initial spectral data of the ZS operator are calculated from the solution which is known at time zero. The spectral data evolve in a trivially simple way, and the remaining step is to recover the unknown solution at time  $t$  from the spectral data at time  $t$ , a process known as inverse scattering. In the case of NLS, the required spectral data corresponding to an initial condition that should naturally lead to modulated waves, is hard to calculate. Furthermore, given the instability of the problem it is not clear to what extent the solution is drastically affected by approximations in the calculation. In collaboration with A. Tovbis, we have developed an example in which the derivation of the spectral data is explicit. Then, in collaboration with A. Tovbis and X. Zhou, we have obtained the following results:

1. We have studied, the evolution of the solution as long as no break (see below) occurs.  
We prove the existence and basic properties of the first break-curve (curve in space-

time above which the character of the solution changes by the emergence of a new oscillatory phase) and show that for pure radiation no further breaks occur.

2. We have constructed the solution beyond the first break-time.
3. We have derived a rigorous estimate of the error.
4. We have derived rigorous asymptotics for the large time behavior of the system in the pure radiation case.

The paper with the above results except the asymptotics has been submitted to CPAM. The paper on the long time asymptotics is in preparation.

## Optimization

In collaboration with Lipton and Shipman, we have applied variational methods to the design of two-dimensional dielectric photonic crystal slabs to optimize resonant scattering phenomena. Because resonant behavior is closely connected to the amount of energy transmitted through a slab, we develop the variational calculus for the transmission with respect to the dielectric and magnetic properties of a structure. It is known that sharp dips and peaks in the transmission coefficient occur at frequencies that are near complex Bloch eigenfrequencies of the slab and exhibit resonant scattering behavior.

Resonant behavior is typically associated with defects in the periodic structure of a crystal. One type of defect we study is a periodic channel running through the slab with a period that is large compared to the period of the pure structure. "Channel modes" occur at the higher end of the bandgap. These are scattering states that exhibit high intensity in the channel, and they are a mechanism for the enhancement of transmission. Typically, this enhancement is weak and shows up as a shallow hump in the transmission coefficient. Using the variational gradient of the transmission, we are able to intensify the channel mode greatly by sharpening the transmission anomaly.

Our numerical methods are based on boundary integrals and are therefore suited to crystals consisting of arrays of scatterers with smooth boundaries.

## Technology Transfer

Our 2D BEM code has been used by H. Everitt (ARO and Duke, Physics) and his group who performed physical experiments towards the manufacture of a photonic crystal laser; the resonant frequencies and corresponding quality numbers computed by our code provided crucial help to the experimental work and were in very good agreement with the experimental values.

Our codes on EM calculations with photonic crystal slabs are available to the Army.

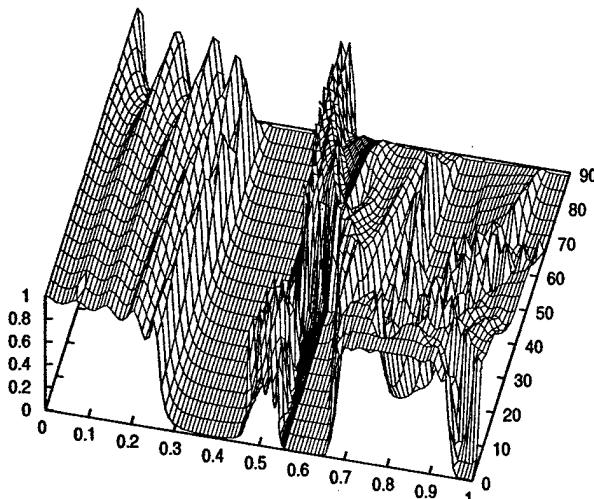
## Publications

1. A. Georgieva, T. Kriecherbauer, S. Venakides, *Wave Propagation and Resonance in a 1-d Nonlinear Discrete Periodic Medium*, SIAM J. Appl. Math. **60** No 1, (1999) 272-294.
2. M. Beaky, J.B. Burke, H.O. Everitt, M.A. Haider, S. Venakides *Two Dimensional Fabry Perot Resonators with Lossy Dielectric*, IEEE Transactions on Microwave Theory, vol. 47 No. 9 (1999) 2085-2091.
3. S. Venakides, M. Haider, V. Papanicolaou *Boundary Integral Calculations of 2-d Electromagnetic Scattering by Photonic Crystal Fabry-Perot Structures*, SIAM J. Appl. Math. **60** No 5 (2000) 1686-1706.
4. S. Venakides, M. Haider, V. Papanicolaou *Wave Propagation in Photonic Crystal Models*, in Proc. 4th International Workshop on *Scattering Theory and Biomedical Modeling and Applications* Ed. G. Dassios, D.I. Fotiadis, K. Kyriaki, C.V. Massalas, World Scientific, 2000.
5. A. Tovbis, S. Venakides *The Eigenvalue Problem for the Focusing Nonlinear Schrödinger Equation: New Solvable Cases*, Physica D **146** (2000) 150-164.
6. A. Georgieva, T. Kriecherbauer, S. Venakides, *1:2 Resonance mediated frequency doubling in a 1-d Nonlinear Discrete Periodic Medium*, SIAM Jr. Appl. Math. **61** No 5 (2001) 1802-1815.
7. M. Haider, S. Shipman S. Venakides, *Boundary-Integral calculations of 2D EM scattering in infinite photonic crystal slabs: Channel defects and resonances* SIAM J. Appl. Math. **62** (2002), 2129-2148.
8. S. Shipman and S. Venakides, *Resonance and Bound States in Photonic Crystal Slabs*, SIAM J. Appl. Math. (preprint 2002) SIAM J. Appl. Math., in press.
9. A. Tovbis, S. Venakides, X. Zhou, *On Semiclassical Solutions of the Focusing Nonlinear Schrödinger Equation* CPAM, submitted.
10. A. Barnes, S. Shipman and S. Venakides, *Scattering and resonance in 3D photonic crystal slabs via a boundary element method*, in preparation
11. R. Lipton, S. Shipman, S. Venakides *Optimization of Resonances in Photonic Crystal Slabs*, Annual SPIE meeting in San Diego (Aug. 3-8, 2003), program on Physics, Theory, and Applications of Periodic Structures in Optics II.

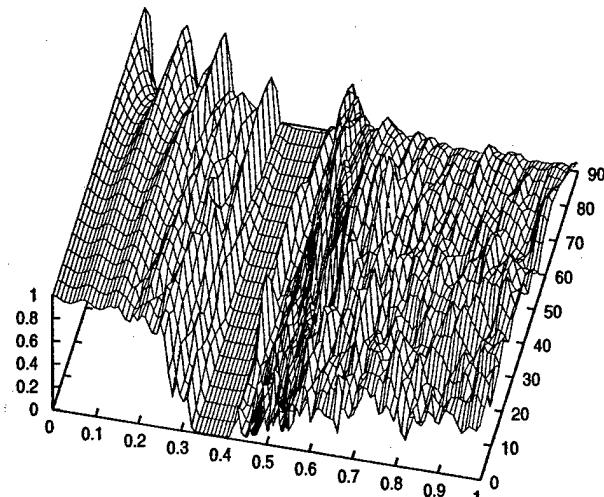
## **Scientific Personnel/Collaborators**

1. Stephanos Venakides (PI), Duke U.
2. Andrew Barnes, Graduate student, Duke U., (will defend PhD dissertation in Sept. 2003).
3. Anna Georgieva, Novartis.
4. Christopher Hale, Graduate student, Duke U., (scheduled to graduate in the academic year 2003-2004).
5. Mansoor Haider, NCSU.
6. Thomas Kriecherbauer, U. Bochum, Germany.
7. Robert Lipton, LSU
8. Vassilis Papanicolaou, NTUA, Greece.
9. Stephen Shipman, LSU.
10. Alexander Tovbis, UCF.
11. Xin Zhou Duke U.

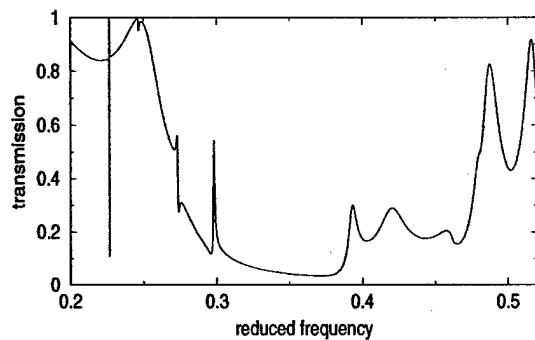
## Appendix 1



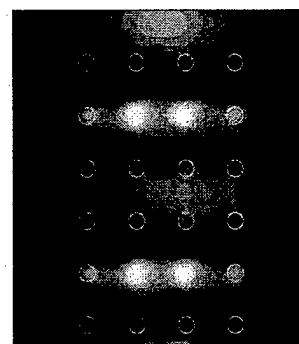
Transmission at all angles of incidence through a perfect square-lattice crystal of circular rods, five rods thick.



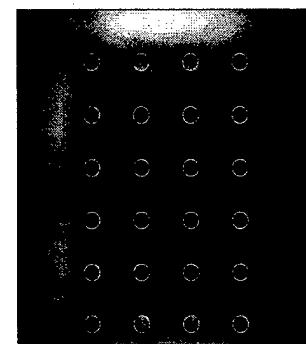
Transmission at all angles of incidence through a square-lattice crystal of circular rods, five rods thick, with randomly perturbed centers.



Transmission at normal incidence through a slab four rods thick, with a periodic channel after every six rows.



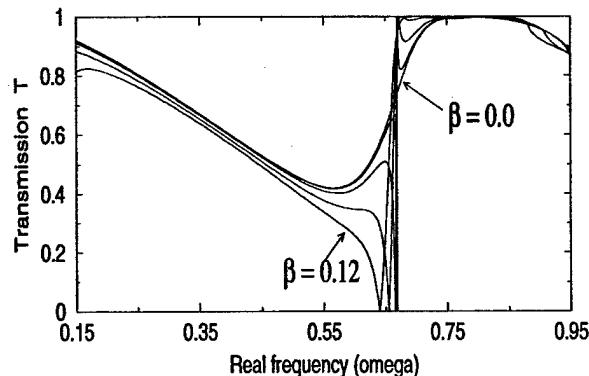
A scattering state at the frequency of the narrow spike at about 0.226.



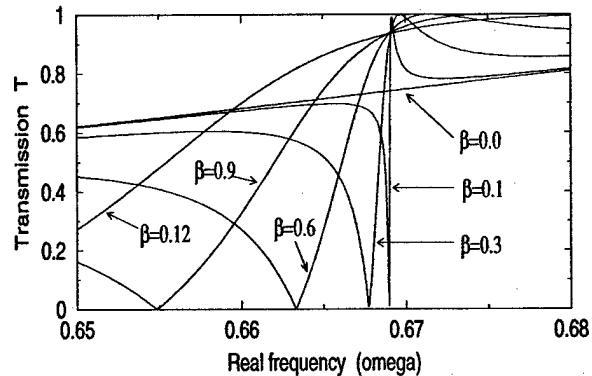
A scattering state at the frequency of the peak at about 0.39.



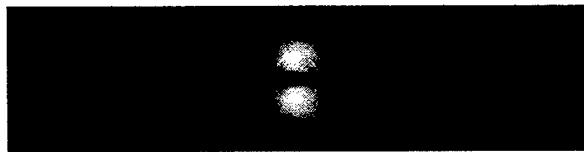
A bound state on the surface of a square-lattice PC in which the first rod is enlarged (one period in the vertical direction is shown).



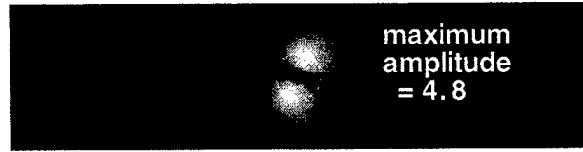
Transmission through a single string of rods at angles close to normal incidence.



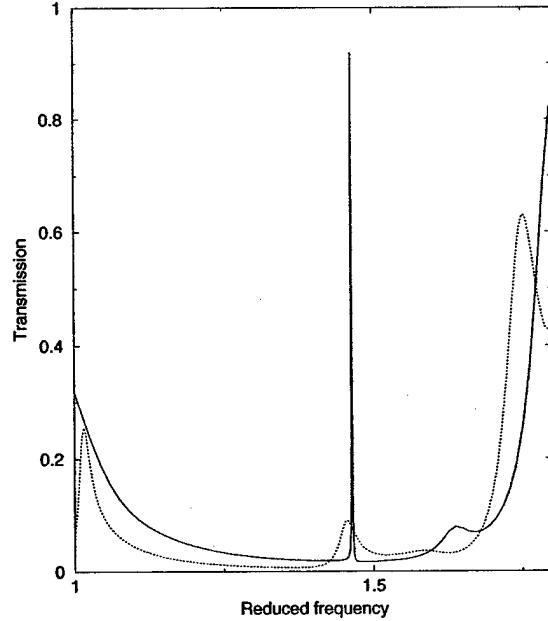
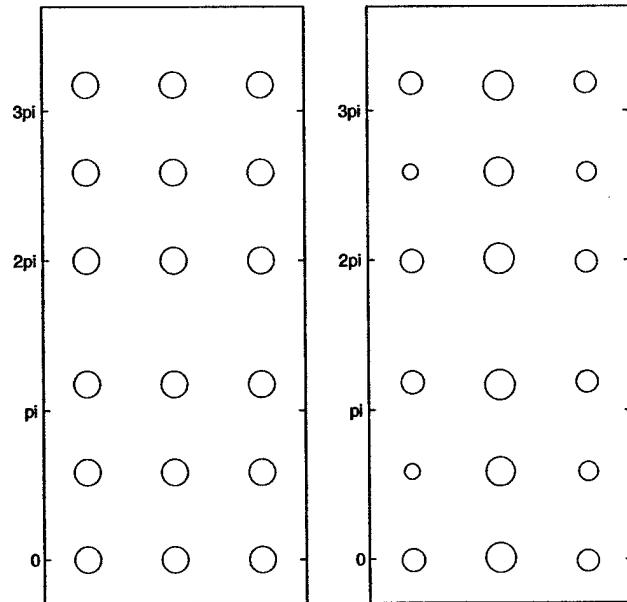
A closer view near the transmission anomalies for several values of the Bloch factor  $\beta$ .



A bound state at  $\beta = 0$ ,  $\omega \approx 0.669$ .



A scattering state at  $\beta = 0.12$ ,  $\omega \approx 0.660$ .



Optimization of resonance: Two periods of a photonic crystal slab (first panel) and the modified slab (second panel). The transmission coefficient of the original slab is shown as a dotted curve and that of the modified slab as a solid curve. The modification is the result of applying the variational calculus to transform the shallow hump into a sharp resonance.